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WHAT BARRIERS PREVENT ICME FROM BECOMING PART OF THE DESIGNER'S TOLLBOX? (PREPRINT)

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Metals Branch

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14. ABSTRACT
Integrated computational materials engineering methodologies promise a revolutionary step forward in the qualification, certification, and sustainment of Air Force systems via reduction of the historically slow and costly materials data development footprint [1,2,3]. The establishment of scientifically-based, statistically-robust processes by which computational materials models can be quantitatively graded, accepted and utilized by the aerospace structures design, manufacture, and sustainment communities for cost and time savings presents a major hurdle towards the realization of the potential of ICME. To allow for the change to the materials qualification paradigm offered by ICME, several barriers (economic, cultural, and technical) must be overcome. Via identification and discussion of these issues, this article challenges the ICME community to position itself for success via integration with the industrial structural design community.

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WHAT BARRIERS PREVENT ICME FROM BECOMING PART OF THE DESIGNER'S TOOLBOX?

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Keywords: Validation, Design, Model, Accuracy, Precision, Culture

Abstract

Integrated computational materials engineering methodologies promise a revolutionary step forward in the qualification, certification, and sustainment of Air Force systems via reduction of the historically slow and costly materials data development footprint [1,2,3]. The establishment of scientifically-based, statistically-robust processes by which computational materials models can be quantitatively graded, accepted and utilized by the aerospace structures design, manufacture, and sustainment communities for cost and time savings presents a major hurdle towards the realization of the potential of ICME. To allow for the change to the materials qualification paradigm offered by ICME, several barriers (economic, cultural, and technical) must be overcome. Via identification and discussion of these issues, this article challenges the ICME community to position itself for success via integration with the industrial structural design community.

Introduction

The development of a fully integrated computational materials engineering (ICME) based structural materials technical field is within reach and its impact upon the aerospace engineering & manufacturing practice and the United States Air Force promises to be profound. Both the aerospace community and the Department of Defense have invested heavily in and developed technically and legally robust structural design, certification, and sustainment processes [4,5,6,7]. Historically, to be integrated into aerospace structural design and life analysis systems, materials were required to undergo millions of dollars (and multiple years) of standardized mechanical testing. The intent of this testing was to develop statistically significant representations of the materials' behavior to independent, but complimentary, combinations of material, manufacturing, and load spectrum combinations. Clearly, ICME presents the opportunity to replace a large degree of historically required mechanical testing providing for faster, less costly design and materials integration cycles. Furthermore, ICME methodologies will enable "transparent" materials and processes substitutions/improvements without the required regeneration of exhaustive materials datasets. To achieve this goal, the materials scientist and engineer community must be cognizant of barriers facing the implementation of ICME in structural design. Economic, cultural, and technical barriers exist. It is the materials community's responsibility to ensure that these barriers are overcome by working to address them in its research, development, and transition activities.

Discussion

<u>Economic Barriers</u>: The cost and time invested in the development of current aerospace design practices and the generation of the supporting materials datasets present a significant barrier to the acceptance of ICME. The economic justification to pull industry toward ICME and invest in new design practices must be cultivated. It is widely recognized [1] that

significant investment must be undertaken to facilitate integration of ICME tools into structural aerospace design. The likely quickest path to overcome this barrier is by the demonstration of point successes (cost and time savings) that can be delivered by ICME. By this mode, examples of ICME acceptance/application in design and manufacture are becoming more frequent [8,9]. The majority of these recent efforts, however, are noted to have been necessitated by time and cost constraints in component development or production driven by unexpected difficulties that did not allow traditional approaches to be utilized. As an emergency stopgap, ICME has been successfully applied in such instances and has been observed to have developed preliminary footholds in specific companies. As a whole, however, confidence must still be established with the structural design community to the extent that the replacement of existing culture and organizational/process infrastructure can be economically justified.

Cultural Barriers: Cultural barriers also present themselves with the integration of ICME into design. Design currently optimizes shape based upon functional requirement (rotating turbine disk, wing spar, etc...), anticipated load spectrum, and materials properties linked to a fixed composition and a correspondingly fixed manufacturing path. Materials are treated as an oversimplified fixed variable in the design optimization process with "shape" being the principal outlet of designer creativity and innovation. ICME presents designers with the opportunity to treat materials as true variables where such concepts as tailoring to achieve location specific properties presents the opportunity for extended creativity where material property can vary with 3-D location in a component. Unfortunately, the addition of materials as an independent variable is a radical departure from current work practice. Such flexibility will push designers into areas where they have neither formalized training, nor corresponding materials backgrounds. It will fall on the materials community to support this re-education of the design community. The path toward ICME implementation in industry will necessarily require a merging of mechanical engineering and materials science and engineering disciplines at this hand-off point.

Technical Barriers: While the economic and cultural barriers faced by ICME are not insignificant, they may not be within the power of all materials researchers to influence. There are, however, multiple global technical barriers that must be addressed to garner the confidence and acceptance of the design community. These barriers include:

- The 'goodness' of current industry practice is accepted, but is not well statistically quantified with respect to materials.
- The accuracy, precision, and error in integrated modeled system predictions are generally not statistically quantified making model predictions difficult to globally accept.
- The ranges over which model predictions are "accurate" are usually not defined, let alone addressed in integrated systems of models.
- "Research" model maturity issues hinder the credibility of computational modeling as a developed technology in the eyes of the structural design community.

The following discussion of these global technical issues is presented to generate thought for researchers developing ICME tools. Without keeping these barriers in mind when developing computational models and presenting their results, materials researchers will not see the transition of their activities to the serve the very needs their research sets out to address.

The complexity of the development of computational models, the verification that such models accurately represent the underlying mathematics models, and confirmation that such models reflect the reality of actual behavior is immense and has been well addressed elsewhere [10].

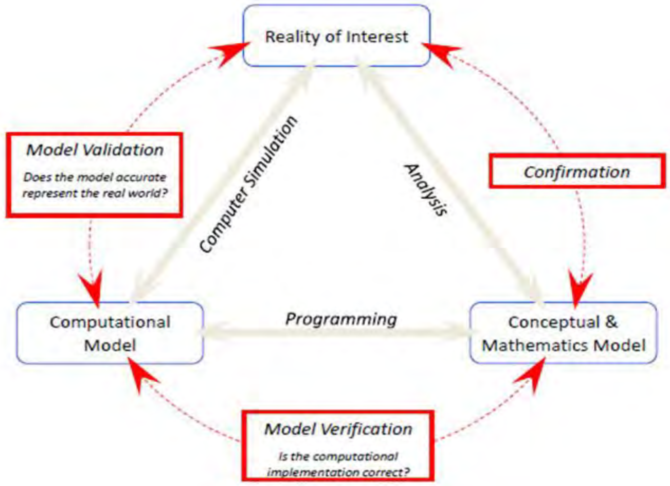

Figure 1. Verification and validation computational model cycle [11].

This discussion will focus specifically on the validation of computational models and the integrated modeling suites (process-microstructure-behavior) to support the aerospace design community (Fig 1.). Validation is defined [12] as, "*the process of determining the degree to which a model is an accurate representation of the real world* *__from the perspective of the intended uses of the model__*." Underlined are the key subjective words in this definition. The design community's perspective and needs are those that materials researchers must ensure are able addressable as their models are presented for validation.

Globally, ICME model validation strategies have not been pervasively established [13]. To enhance the acceptance of ICME by the design community and support the development of validation methodologies, the materials community must begin to look at ICME from the designer's perspective and be prepared to address some of the following questions:

What Is "Goodness" In A Designers Eyes?

US Air Force design is focused on driving the probability of catastrophic field failure to less than one in ten million (0.00001%) [14]. Such failure rates and the current design infrastructure have been validated by field experience. Unfortunately, while the conservative failure goals are well defined statistically, the assumed materials contribution is not probabilistically defensible. To meet probabilistic system failure rate goals, materials are assumed to have normal behavior distributions and their -3σ properties are typically utilized from these distributions as 'safe' design values [15] for critical components. It is therefore this probability of failure (0.15%) that is rolled into the structural design calculation as the materials contribution. This approach appears sound at first review, but implicit to this approach is the fundamental assumption that the property data collected is, in fact, the "worst case" distribution of properties, exercising the limits of specification chemistry, manufacturing process control, and mechanical test variability. Furthermore, the assumption that all behaviors (even those structurally driven) act as normal distributions is clearly not a universal truth. Current, US Air Force airframe structural integrity practice also adds an additional layer of conservatism (an assumed initial flaw) to account for "unexpected" manufacturing anomalies not captured in the development of design data as a response to historical aircraft mishaps [16]. This approach has served the US Air Force well, however, the direct application of this somewhat flawed approach toward acceptance of ICME generated probabilistic results presents real problems for the materials community.

An ICME prediction of mean behavior alone is insufficient for use in probabilistic design. A useable computational prediction of material behavior must address the shape and tails of behavior distribution curves. An ICME framework with validated ability to model chemistry, manufacturing processes, resulting microstructure, and predicted behavior presents a double edged sword of opportunity for the design community. In its best case, a well modeled material may show a distribution with -3σ behavior higher than the traditional dataset. If accompanying high confidence manufacturing process modeling could convince designers to remove the assumed initial flaw assumption, substantial weight savings, or load capacity could be recovered. In its worst case, however, accurate modeling of extreme behavioral outcomes from the material and processing path may show the historical design data based assumptions to be unconservative. Clearly, this result could drive increased inspections of fielded aircraft or fleet groundings if applied to legacy systems, unpopular outcomes to say the least. The materials community must seek to address the technical issue of delivering results that can be incorporated into probabilistic design, but at the same time be cognizant of the implications that may result and designer hesitancy to move forward too quickly.

How Should Model Accuracy and Precision be Addressed?

Qualitative comparison of model prediction to experimental data has become typical for research model validation. Modeled curves of similar shape, slope and data overlap are clearly indicative of "goodness", but are often not quantified. To a designer, such subjective analysis is unusable. The issue at hand becomes comparison of experimental behavior mean curve (with distributions at each point) with model predicted mean curves and distributions in a statistically robust manner. Until such methodologies for model evaluation for accuracy and precision are developed and promoted by the materials community, the design community cannot be expected to establish acceptance criteria for model performance.

Implicit to any statistical analysis of model prediction to actual experimental behavior is detailed knowledge of the exact materials pedigree (chemistry, process history, resulting microstructure, etc…) as well as experimental conditioning. Unfortunately, details of much of the required pedigree information do not exist for historical datasets. Historical mechanical behavior dataset development required only knowledge that the material tested was produced to appropriate specifications and did not capture the specifics that models will eventually be able to address in detail. The true evaluation of model quality must include experimental results from materials whose exact pedigrees (including such things as chemistry, processing strains, strain rates, temperature, etc…) can be linked to the predictive models exercised.

In addition to statistical "fit" analysis, further quantification of a model's accuracy and precision can developed by the modeling of similar and degeneratively simplified problems [10]. Demonstration of successful, high quality prediction of behavior of simplified devolved (subset) problems will add credibility to any result. Likewise, the systematic use of sensitivity [17] tests to evaluate model response to small changes in inputs and assumptions will give insight into model stability and even identify limitation issues.

Complicating the model accuracy barrier even further are the instances where models attempt to predict phenomenon that there are no trusted (or high quality) experimental techniques. In these instances, the role up of these models into larger scale models where validation can occur is the most sensible approach. The tracking of error roles into that of the larger scale model and must be accounted.

What is the Range Of Accuracy of the Models (and can they be Extrapolated?)?

Once a methodology is established to compare model prediction with experiment and designers can quantify and specify required accuracy, boundary value testing can be applied to track model "sweet spots" and bound ranges of accuracy. Models should strive to demonstrate one and only one period of experimental convergence with model prediction as an accuracy range. Multiple, complex regions of accuracy will induce doubt in the eyes of the design community. Similarly, when rolling multiple models into a complex integrated predictive suite, tracking and appropriately managing these ranges of accuracy will be critical and will require materials community driven methodologies to be developed.

Of significant interest to the structural designer are material behavior regimes beyond historical precedent. This exploration is indeed the promised fruit of ICMSE. Such exploration will require extrapolation or use of models beyond where their established range of accuracy. Such extrapolation should only be considered/supported by the materials community in instances where the applied models have sufficient physical basis (non-phenomenological) and have not incorporated any type of calibration. Model calibration (even to physics based models) exhibits lack of confidence in the model by the materials scientist/engineer. It is viewed similarly by the designer! Calibration to achieve agreement in a regime of interest fundamentally corrupts the model's ability to be applied/extrapolated elsewhere with confidence.

Finally, a robust means of holistically evaluating model quality and applicability can be accomplished via the use of benchmarking [18]. By using design of experiments methodologies to produce materials that capture and extend beyond current industrial practice norms (i.e. forged shapes that include both nominal and abnormal plastic deformation, rates, & temperatures) data can be generated to exercise and evaluate model quality outside of normal ranges. During such manufacture, critical 3D microstructural information (chemistry, geometry, texture, and residual stress) could be extracted (as computational models input). Following manufacture, multi-scale mechanical testing can be used to generate statistically robust experimental datasets. Such a benchmark would enable studies of individual models as well as integrated modeling suites for purposes of validation.

Are the Presented Models Sufficiently Developed?

Computational materials model creation and development is thankfully on the rise. A "cottage industry" is developing in both the academic and commercial sector towards this end. It is the author's observation that the combination of funding direction and targeted application is, however, resulting in the development of such models stopping at relatively immature states. When either the problem the model was developed for has been "solved" or the model is subjectively "validated," development often ceases. At this point, significant work has gone into the mathematical model development, code development, and verification that the code represents the mathematical model. Many models, have no documentation on neither their basis nor use and can be generally best be characterized as user unfriendly (if available for use at all). While there are economic and competitive drivers for keeping close hold on certain models, the end effect is often a lack of transition of this work to the community at large. A cursory review of any major university materials department dissertation library will show record of model development and some degree of validation success. The real challenge then becomes obtaining (or gaining access) to the exact model that generated those results. Lack of documentation, revision control and availability of that model then all quickly become significant issues that impede subsequent successful application. The design community will require any supporting model to be developed to such an extent that revision control, underlying assumptions, required inputs, and operation are knowns. The materials community must come to grips with the fact that until models reach this point of development, they will largely not be useable by the design community.

Conclusion

The materials scientist and engineer community must keep in mind the perspective of the design community (their ultimate customer) as they continue to create and develop ICME technologies. The materials community will have to take an active role in the development of methodologies to quantify accuracy, precision, track error propagation, and envelope of model relevance. The materials community must also strive to provide models that are developed sufficiently to transition into integrated computational suites. Only by satisfying the design community's concerns and establishing confidence in the utilization of ICME tools to replace a robust historical paradigm, will a future home for computational materials science technologies be ensured.

References

[1]National Research Council (NRC), National Materials Advisory Board, *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*, Washington, D.C., National Academies Press, 2008

[2] National Research Council (NRC), *Materials Research to Meet 21st Century Defense Needs*, Washington D.C., National Academies Press, 2003

[3] National Science and Technology Council, Fast Track Action Committee on Computational Modeling and Simulation Committee on Technology, *Simulation-Based Engineering and Science for Discovery and Innovation*, Released for Comment, May 2010

[4] Department of Defense Handbook, Aircraft Structural Integrity Program General Guidelines For, MIL-HDBK-1530C, 1 Nov, 2005.

[5] Department of Defense Handbook, Engine Structural Integrity Program, MIL-HDBK-1783B, 15 Feb, 2002.

[6] Department of Defense Joint Service Specification Guide, Aircraft Structures, JSSG-2006, 30 Oct 1998.

[7] Department of Defense Joint Service Specification Guide, Engines, Aircraft, Turbine, JSSG-2007A, 29 Jan 2004.

[8] J. Allison, L. Mei, C. Wolverton, S. Xuming, Virtual Aluminum Castings: An Industrial Application of ICME, JOM, Vol. 58, No. 11, pp. 28-35.

[9] Materials Modeling and Simulation—A Game Changing Technology for Propulsion Materials Development
D. D. Whitis[1], R. Schafrik[2], (1)GE Aviation, Evendale, OH, (2)GE Aircraft Engines, Cincinnati, OH, Aeromat, 2007.

[10] C. Kuehmann, H.J. Jou, "Model Quality Management," ASM Handbood, V22A, Fundamentals of Modeling for Metals Processing, ASM International, 2009.

[11] S. Schlesinger, "Terminology for Model Credibility," Simulation, Vol. 32, No. 3, 1979, pp. 103-104.

[12] ASME Validation and Verification Guide, 10-2006, 2006.

[13] Personal communications with US Air Force supplier base , Air Force Research Laboratory, Materials and Manufacturing Directorate, Closed Verification and Validation Workshop, Feb, 2011.

[14] J.P. Gallagher, C.A. Babish, J.C. Malas, "Damage Tolerant Risk Analysis Techniques for Evaluating the Structural Integrity of Aircraft Structures, " Proceedings, 11th International Conference on Fracture, ISBN 978-88-903188-0-1, March 2005.

[15] DOT-FAA-AR-MMPDS-01, Metallic Materials Properties Development And Standardization (MMPDS), 31 JAN 2003.

[16] Gebman, J. R., "Challenges and Issues with the Further Aging of US Aircraft – Policy Options for Effective Life-Cycle Management of Resources, ISBN 978-0-8330-4518-8, UG1243.G429.2009.

[17] A.V. Fiacco, "Sensitivity and Stability in NLP: Approximation," ENCYCLOPEDIA OF OPTIMIZATION
2009, Part 19, 3454-3467, DOI: 10.1007/978-0-387-74759-0_594

[18] F. Stern, R. Wilson, J. Shao, "Quantitative V&V Of Cfd Simulations And Certification Of Cfd Codes With Examples," Proceedings of CHT-04,ICHMT International Symposium on Advances in Computational Heat Transfer, April 2004.